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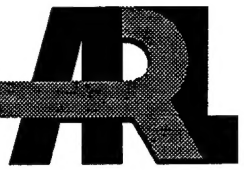

A New Approach to Propellant Formulation: Minimizing Life-Cycle Costs Through Science-Based Design

by Martin S. Miller, Betsy M. Rice, Anthony J. Kotlar,
and Randall J. Cramer

ARL-TR-2291 August 2000

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A New Approach to Propellant Formulation: Minimizing Life-Cycle Costs Through Science-Based Design

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Abstract

The traditional approach to developing propellants for specific gun applications relies heavily on trial and error. Candidate formulations must be made in small quantities and subjected to burning-rate measurements and small-scale vulnerability assessments. If the properties of these candidates fail to meet expectations, the process must be repeated. This approach, while historically unavoidable, is obviously inefficient in time and expense and can generate considerable waste streams associated with unsuccessful formulations. With added considerations of life-cycle costs, including environmental impact at all stages of development, use, and disposal, this traditional approach becomes increasingly unworkable. This report proposes a new approach that makes maximal use of scientific understanding embodied in models during the early phases of the propellant-development cycle. Simple simulations show that this strategy can have a significant impact on the overall costs of the development process. In analogy to the Department of Energy (DOE) program to convert the nuclear-weapon stewardship from testing-based to science-based, we term the new approach science-based design. This new approach will require concentration and leveraging of resources toward the most critical early-phase development steps; with the reality of declining resources, it may be the only credible strategy to reconcile the need for higher-performance weapons.

Acknowledgments

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1. Introduction

The recent Quadrennial Defense Review [1] discussed the challenges faced by the Department of Defense (DOD) in realizing the new support structure needed to achieve the future military forces outlined in the Joint Vision 2010 document [2]. In order to afford the increasing expenditures associated with these new capabilities, the QDR concluded that support operations must be "leaner, more efficient, and more cost effective. We not only have the opportunity to change, we have the requirement to change." Nowhere is this mandate more apt than in the development of new propellant formulations for advanced munitions. In the past, development has been dependent on trial and error approaches, which are costly, inefficient, and time consuming. Compounding these problems are new environmental guidelines and constraints with which future development programs must comply. Since conventional propellant development and manufacture produces large amounts of waste, these new requirements could hobble the process. During the development of XM39 gun propellant during the 1980s, for example, about 50,000 lb of test material was produced [3], almost all of which was waste resulting from the trial and error testing required. During the current manufacture of M30 gun propellant, an estimated 0.3 lb of ethanol and acetone are released to the atmosphere for every pound of propellant [4]. These examples hint at the scale of potential environmental hazards that now must be addressed. As more performance is demanded from gun systems, the margin for error in their design decreases, leading to even greater levels of trial and error during development. Clearly, the added modern burden of environmental responsibility will render the traditional approach to propellant development even more unmanageable.

The new environmental constraints are not trivial add-on requirements. They encompass the manufacture of every ingredient, fabrication of the propellant itself, emissions in training and deployment, stability during storage, and demilitarization when no longer useful. Design foresight on issues relating to storage (stability surveillance and emissions) are of great potential importance since the useful life of propellants can be long; 16-in naval guns, for instance, still use a propellant known as pyro, which was manufactured during (or just after) World War II. Propellants are also manufactured in large quantities; a single batch of artillery propellant is typically more than a hundred thousand pounds. Thus, the cradle-to-grave costs associated with propellants, both to the

national treasury and to the environment, are potentially very substantial. While assessing life-cycle costs for a new propellant is difficult, managing these costs using the traditional trial and error development method is all but impossible. It is argued in this report that the conflict between the need to develop advanced propellants for more lethal, survivable weapons and the need to minimize life-cycle costs can be resolved only by a new approach. Just as new realities have forced the maintenance of the nation's nuclear stockpile to pass from a testing-based to a science-based approach, developing new propellants must transition from a trial-and-error-based to a science-based approach.

Fortunately, the scientific understanding of the microscopic processes involved in the structure and combustion of energetic materials has seen great progress over the last decade. Although this understanding is far from complete, sufficient progress has been made to permit a vision of how new tools for the smart design of propellant formulations might be used to minimize inefficiencies in the propellant formulation process. Such an exercise is also valuable in identifying those key aspects of the problem where investments in future scientific understanding might be made most profitably. The ideal developmental process utilizing these emerging technologies will incorporate the constraint of reducing the waste streams resulting from all the stages of fielding a new propellant with preserving the given performance objectives, which are the *raison d'être* for the process. This report will outline such a streamlined development approach.

2. Traditional Propellant-Formulation Process

The traditional procedure for formulating new propellants, guided largely by intuition, experience, and testing, relies heavily on trial and error. Candidate propellant mixes must be made and subjected to a sequence of tests, many of which generate hazardous emissions and wastes. In addition to the waste generation associated with test and evaluation, many of the candidates are discarded from further consideration due to unacceptable levels of performance or other problems that arise in the qualification procedure. For these cases, waste costs accrue for unsuccessful formulations, synthesis and testing, and disposing of any excess material. It is clear that such cut-and-try approaches, although previously unavoidable, are now considered inefficient, costly, and environmentally undesirable.

Figure 1 illustrates the conventional process of developing a new propelling charge. This flow chart presumes that adequate ingredients (e.g., energetic materials and polymeric binders) are "on the shelf" to achieve a successful formulation. If this is not the case, then new ingredients with the desired characteristics must be developed. Before embarking on the procedure outlined in Figure 1, the weapons designer will have specified his requirements, which in the past have been driven mainly by performance or vulnerability requirements. The initial screening represented by Loop 1 consists of computations of impetus, flame temperature, and idealized maximum performance based on thermodynamic equilibrium, which may be viewed as a limiting case. At this stage, a formulation can be rejected if it cannot meet performance needs, even assuming a theoretical maximum performance. If a candidate passes this level, however, shortfalls from theoretically ideal performance revealed at subsequent levels may yet cause it to be rejected, in which case the burden falls back on the formulator to provide a new candidate to run the gauntlet of screening tests from the beginning. (Note: In this flow chart and those to follow, a very complex process is rationalized into a limited number of discrete steps. Such an idealization is necessarily oversimplified and is intended to serve only a heuristic purpose.)

Once the small-scale evaluations are made, then more extensive tests and measurements are performed for increasingly larger samples. As evident in this figure, the conventional method has a notable degree of physical testing and measurement, which could generate a significant amount of waste. Although the small-scale screening procedures contained within the first four loops are relatively inexpensive on a per-sample basis in terms of time, material, and equipment requirements, these might become quite cost intensive if a series of failures require reformulating and retesting several candidates. Because of the nested nature of these screening loops, an inexpensive single-step operation could make the formulation procedure cost prohibitive.

As an illustration of the potential expense associated with the repeated execution of the innermost loops resulting from the traditional trial and error approach to propellant formulation, consider the following fictitious case of a gun-propellant development. To determine the expense associated with developing a new propelling charge, costs were assigned to each stage of the formulation procedure outlined in Figure 1. Naturally, these costs will vary enormously in

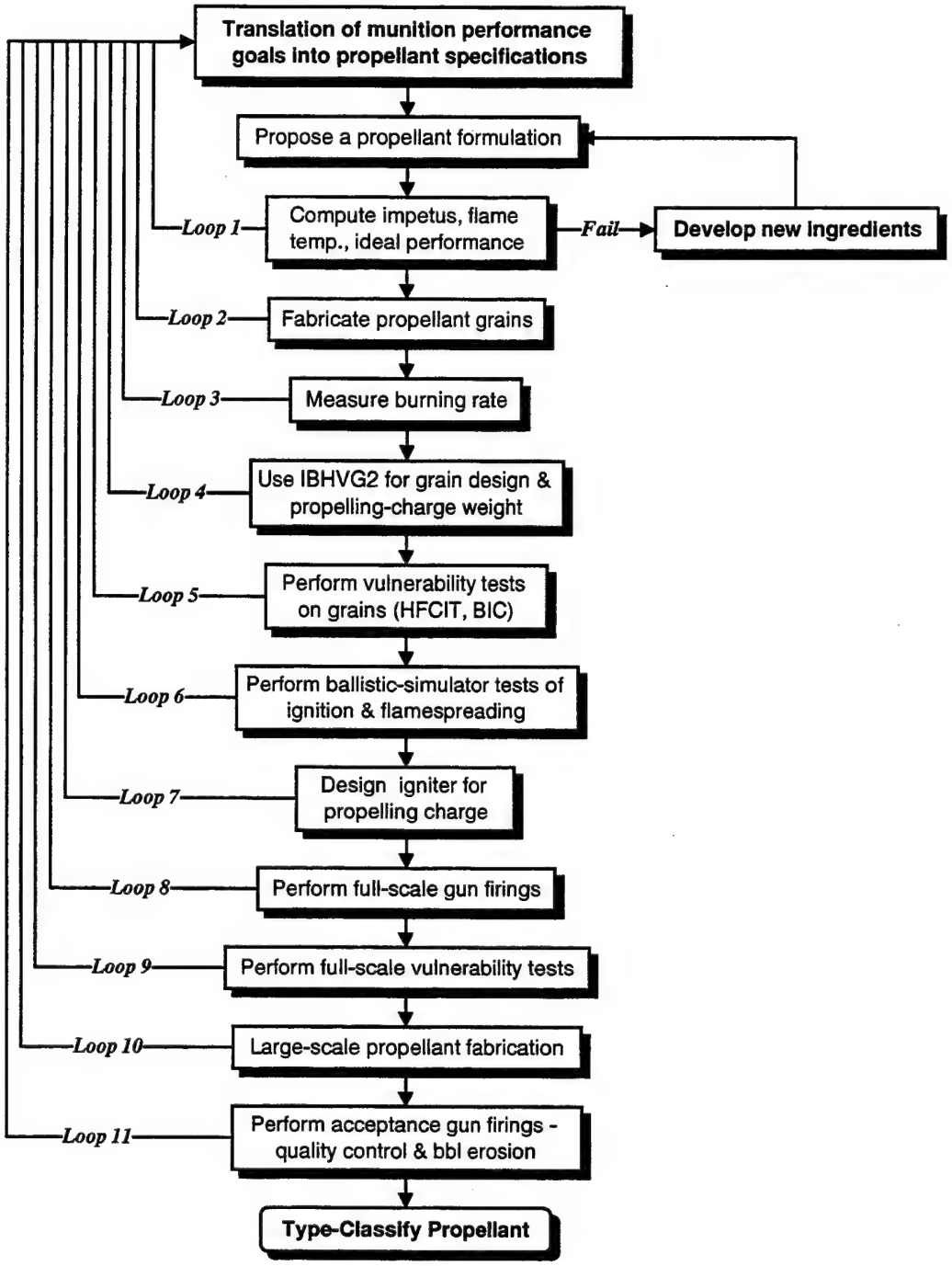

Figure 1. Conventional Procedure for Development of a New Propelling Charge for Guns.

actual cases, but an effort was made to make reasonable estimates for these steps. These numbers should be taken within their intended heuristic context and not taken literally. The relative values assigned are intuitively reasonable in that the early "screening" processes are the least expensive, and

the large-scale processes reflect the more significant costs of the procedure. For the purposes of this illustration, it was assumed that the formulator did not require new energetic material synthesis.

In this exercise, it was assumed that the progression through the entire process would require three passes through each loop in Figure 1. In reality, of course, each loop will incur a different number of executions uniquely specific to each propellant-development case. The value of choosing a single number for all loops is purely in the simplicity and transparency it confers to the simulation. The selected value of three passes is arbitrary, but it reflects the reality of at least some degree of trial and error.

The results of this simulation are given in Table 1. In this simple example, three-fourths of the total cost occurs in the first three stages of the developmental process through steps that, when individually taken, are at three to four orders of magnitude less expensive than the processes near the end of the developmental process. This result is dramatic evidence of the enormous hidden costs associated with trial-and-error testing at the early development stages. In actual practice, the total costs incurred by this inner-loop testing have never been this large, only because a complete matrix of testing would be prohibitive. The thoroughness of the formulation search was therefore consciously curtailed. Undoubtedly, the incompleteness of the search jeopardizes optimization of the formulation. Another reason that such inner-loop costs have never been this large is that performance requirements would have been sacrificed at an early stage to keep costs down. This downgrading of expectations could have easily compromised the maximum attainable performance had more complete testing been feasible.

The inefficiencies inherent in the trial-and-error approach may have consequences beyond exorbitant monetary cost. In the modern era of warfare, a great premium is placed on agile response capability to new threats. There could be occasions where protecting some strategic asset is worth virtually any expenditure, yet the time needed to extensively test may prove to be the pacing limitation. An example of the time needed to develop a new propellant can be seen in the case of M43, a high-performance tank-gun propellant. M43 was under development for almost 20 years before being type classified shortly before Operation Desert Storm. In this case, the presence of an untried propellant ingredient, cyclotrimethylenetrinitramine (RDX), may have materially lengthened

Table 1. Demonstration of the Multiplier Effect Associated With Repetitive Executions of Low-Cost, Inner-Loop Steps in Traditional Propellant-Formulation Procedure of Figure 1

Loop No.	Per-Loop Cost ($K)	Total No. of Times Executed During Entire Procedure	Total Cost of This Step Through Entire Procedure (Total No. of Times Executed × Cost/Loop) ($K)
1	3	3^{11} = 177,147	531,441
2	5	3^{10} = 59,049	295,245
3	2	3^{9} = 19,683	39,366
4	5	3^{8} = 6,561	32,805
5	5	3^{7} = 2,187	10,935
6	40	3^{6} = 729	29,160
7	10	3^{5} = 243	2,430
8	300	3^{4} = 81	24,300
9	100	3^{3} = 27	2,700
10	3,000	3^{2} = 9	27,000
11	50,000	3^{1} = 3	150,000
Total Cost			1,145,382

the process. But instead, this lack of experience simply increased the number of iterations of testing needed to assure the safety and consistency of the new propellant. Obviously, there may likewise be cases where the environmental consequences of a particular propellant or ingredient may be so egregious that cost and time become of secondary importance.

3. The Impact of Life-Cycle Analysis on Propellant Formulation

The need to minimize the waste associated with the propellant formulation process is no longer driven purely by monetary constraints. Environmental restrictions and requirements have demanded

that environmental impact be given equal or greater weight in the development and design of a new gun propellant. Along with increasingly important environmental considerations has come a focus on the true cradle-to-grave costs of weapons systems. Optimizing the design of a system to minimize development, manufacturing, and operational costs is a considerable challenge. Now, the cost of demilitarizing the system at the end of its useful life must also be included. In the past, propellants have been disposed of by open-air burning. In the future, this method of disposal may not be allowed. Therefore, considering how the propellant will eventually be destroyed or recycled will have to be included in its design. The collective cradle-to-grave costs, including environmental considerations at each stage of manufacture, use, and disposal, have been termed life-cycle costs.

To account for these requirements, the propellant formulation procedure must be modified to reflect these new design considerations. Figure 2 suggests how the inclusion of environmental constraints (Loops 2 and 6) might modify the conventional propellant-development flow chart (Figure 1). The simulation logic of Table 1 assists in estimating the added burden on the propellant development process introduced by the environmental considerations. In the modified simulation shown in Table 2, very modest per-loop costs are assigned to the environmental steps. A substantial increase in total cost results from adding only two new steps. Even if it is assumed that these two environmental steps cost nothing, the total cost of the development sequence is increased by a factor of five. Obviously, adding environmental constraints can easily overwhelm the practicality of the traditional cut-and-try development method. Greater rationalization of the early steps in the propellant-development procedure is clearly needed to successfully manage this added complexity.

4. Propellant Formulation Through a Science-Based Approach

Prior to the ban on underground nuclear weapon tests, the Department of Energy (DOE) used direct tests to regularly test design concepts and the safety and reliability of nuclear weapons in the strategic stockpile. With the cessation of testing, these concerns had to be satisfied through computation based on a reliable scientific understanding. This strategy is embodied in what is called

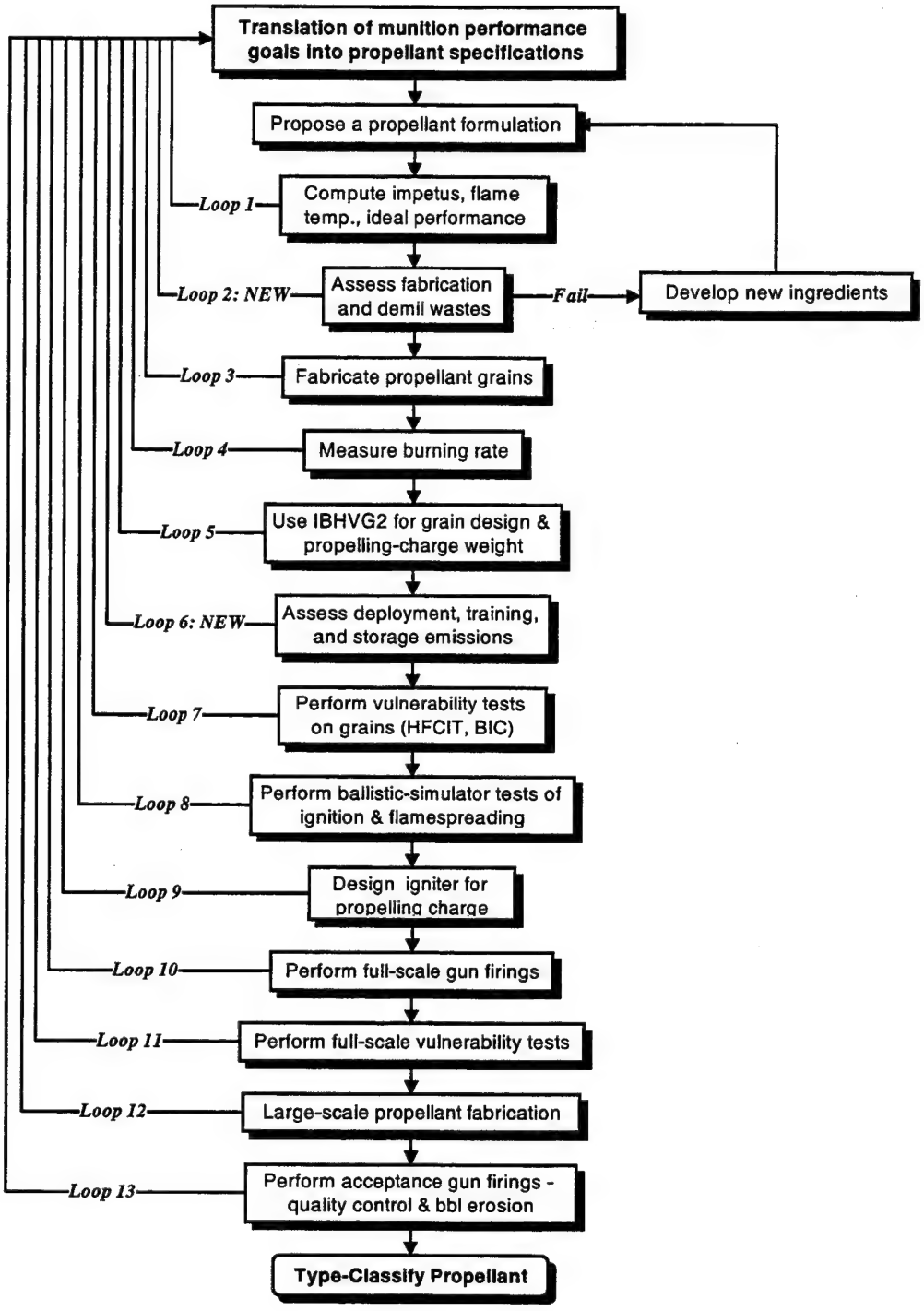

Figure 2. Conventional Procedure for Developing a Propelling Charge With the Addition of Two New Loops (2 and 6) Recognizing Environmental Constraints.

Table 2. Effect on the Total Cost of Development of Including Two Environmental Steps Into the Traditional Propellant-Formulation Procedure (Figure 2)

Loop No.	Per-Loop Cost ($K)	Total No. of Times Executed During Entire Procedure	Total Cost of This Step Through Entire Procedure (Total No. of Times Executed × Cost/Loop) ($K)
1	3	3^{13} = 1,594,323	4,782,969
2	2	3^{12} = 531,441	1,062,882
3	5	3^{11} = 177,147	885,735
4	2	3^{10} = 59,049	118,098
5	5	3^{9} = 19,683	98,415
6	4	3^{8} = 6,561	26,244
7	5	3^{7} = 2,187	10,935
8	40	3^{6} = 729	29,160
9	10	3^{5} = 243	2,430
10	300	3^{4} = 81	24,300
11	100	3^{3} = 27	2,700
12	3,000	3^{2} = 9	27,000
13	50,000	3^{1} = 3	150,000
Total Cost			7,220,868

a science-based stewardship. This term is not meant to imply that science was not formerly used; however, now the burden to assure an accurate, detailed understanding of the microscopic processes is acute, as total reliance is being placed on it. The DOE has redirected funds formerly used in testing into experiments and theory designed to bolster gaps in fundamental understanding of phenomena related to design and aging issues. While testing in the development of propellants is permissible and important, it is expensive in dollars, time, and environmental impact. The propellant-formulation community could profitably adopt the spirit of the DOE science-based strategy.

Efforts to develop predictive technologies leading to smart design have been underway for several years within DOD mission programs. These efforts include developing molecular-dynamic models [5–7] of RDX (and CL20) structure and aggregate properties, theoretical tools [8] for predicting the stability and heats of formation for notional energetic materials, models [9] to predict the burning rate of a propellant from its ingredients, and models [10, 11] to compute the effects of finite-rate kinetics on flame spreading in a propelling charge. These emerging predictive technologies can form the basis of the science-based approach to propellant development, which can in turn minimize the cost of the propellant formulation procedure by reducing synthesis and measurement. Unfortunately, these efforts have focused almost solely on performance, without regard to environmental hazard. A continued and leveraged effort to develop these capabilities to incorporate environmental constraints should be undertaken.

To minimize propellant-development costs (whether they be monetary, time, or environmental), the developmental procedure must be optimized. Such an optimization can be achieved if:

(1) the number of times the inner loops are accessed is minimized, and

(2) the processes included in inner loops are either eliminated or made as cost efficient as possible.

These two requirements for achieving optimization can be met by extensively utilizing modeling and simulation. Results from modeling and simulation provide the insight needed for the smart design of materials. Modeling and simulation are relatively cheap and fast. There is no need to fabricate test material and no need for the labor and expense of manning and maintaining test equipment. Additionally, there is no expense associated with hazardous material, including synthesis, handling, cleanup, or disposal costs.

Figure 3 shows a flow diagram attempting to optimize the propellant formulation procedure by replacing early-phase testing and measurement with modeling and simulation. Continuing in the spirit of the two simulations previously mentioned, it was assumed that a model for predicting the

burning rate has been developed and that it was incorporated into Loop 1. The capability to compute the burning rate would obviate the need for fabricating propellant grains for the burning rate measurement and the measurement itself. Next, it was assumed that vulnerability models exist that can at least screen candidates at the Loop 1 level. Finally, it was assumed that models exist that can predict flame spreading and igniter functioning well enough to eliminate the testing associated with these steps and incorporate these functions into Loop 4. The per-loop execution cost in Loops 1 and 4 was increased to reflect the added modeling effort. These activities are all areas of active research under mission programs of the U.S. Army Research Laboratory (ARL) and have realistic chances for success.

The results of this simulation are given in Table 3, and they show a dramatic drop in total development costs by a factor of almost 30. Notice that the new emphasis on smart design returns the heaviest cost burden to the large-scale testing and acceptance firings. Concern over troop safety will always demand extensive quality assurance testing at this end of the development cycle. Modeling and simulation are most effectively used in the beginning stages of the development cycle. These numbers are not intended to be taken too literally. The total costs are obviously a function of the number of steps in each chart, and the degree of simplification inherent in these charts does not permit them to be unique. On the other hand, the concept behind the numbers is sound. Adding environmental constraints unambiguously adds steps to the development process, which increases costs. Innermost loop functions are exercised the most and are the most susceptible to having testing replaced by models. Replacing relatively expensive testing with relatively inexpensive models leads to either total elimination of inner-loop steps (such as propellant fabrication for burning-rate tests) or consolidated inner-loop functions. The end result is an unambiguous reduction in money, time, and environmental impact.

5. Implementation

The simplified flow charts illustrate the nested-loop nature of the propellant-development process and the total cost reduction that will be realized by modeling various combustion characteristics and

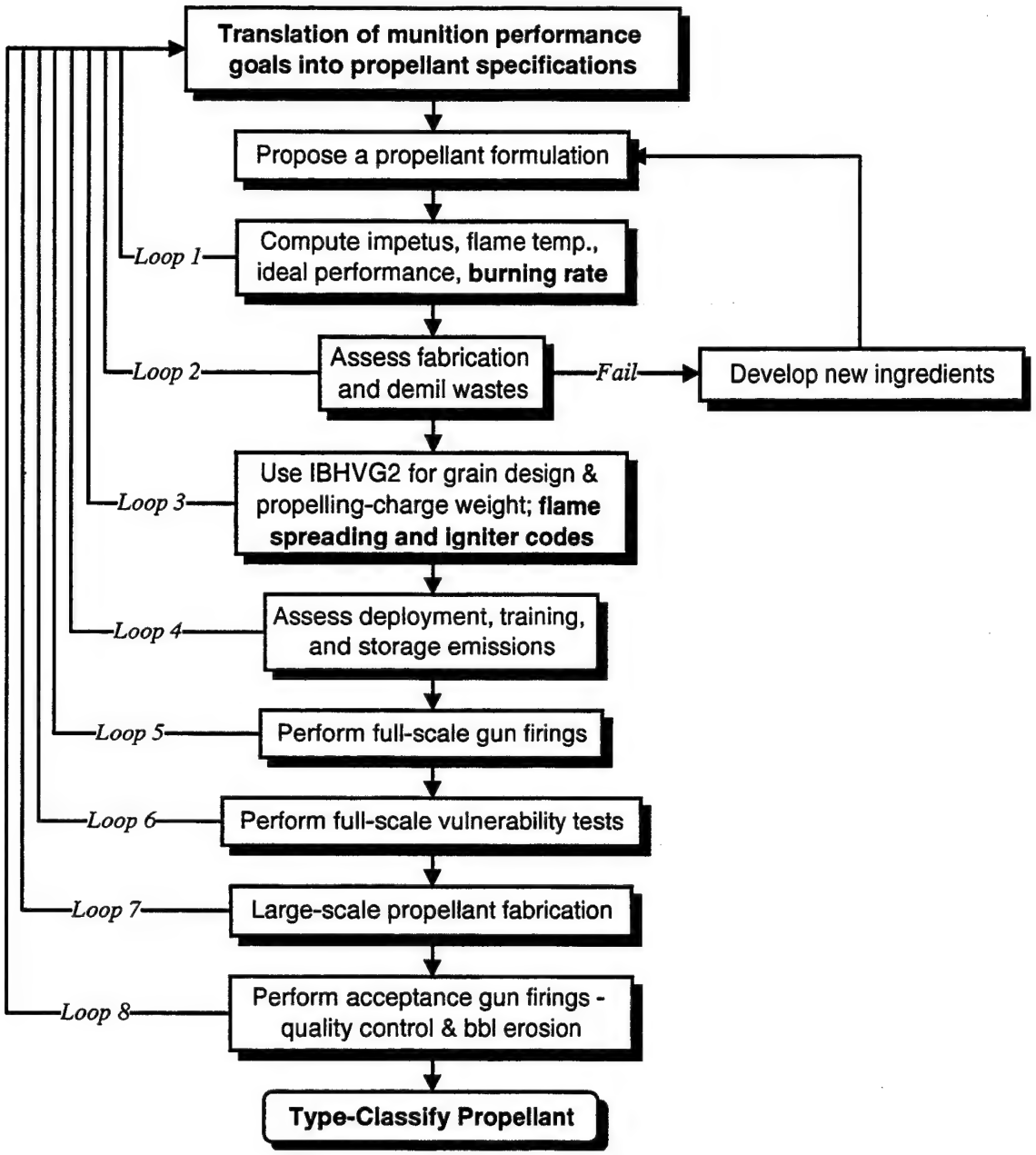

Figure 3. Streamlined Propelling-Charge Development Utilizing Modeling During Early Phases.

Table 3. Effect of Streamlining the Propellent-Formulation Procedure Through the Use of Modeling and Simulation (Figure 3)

Loop No.	Per-Loop Cost ($K)	Total No. of Times Executed During Entire Procedure	Total Cost of This Step Through Entire Procedure (Total No. of Times Executed × Cost/Loop) ($K)
1	5	3^8 = 6,561	32,805
2	2	3^7 = 2,187	4,374
3	7	3^6 = 729	5,103
4	4	3^5 = 243	972
5	300	3^4 = 81	24,300
6	100	3^3 = 27	2,700
7	3,000	3^2 = 9	27,000
8	50,000	3^1 = 3	150,000
Total Cost			214,449

behavior. They do not, however, convey the fact that a hierarchy of models exist with differing sophistication and differing requirements for the input information. For example, IBHVG2 is an interior-ballistic code useful in the preliminary design of a propelling charge, but it cannot predict problems with ignition delays arising from finite-rate chemical kinetics. On the other hand, it also does not require chemical kinetic mechanisms as input, as would the more sophisticated XNOVAKTC/NGEN codes. The XNOVAKTC/NGEN codes also consume considerably greater computer resources and require more skill to use properly. Thus, for the optimum candidate, the most efficient approach to sorting through a large number of existing propellants is to use a succession of codes of increasing sophistication. Eliminate as many candidates as possible by using simpler codes first; reserve the more detailed, data-hungry, and operator-intensive codes for the more promising candidates. A flow diagram illustrating this hierarchy of sophistication in evaluation codes is given in Figure 4. References for the computer codes identified in Figure 4 are given in Table 4.

In Figure 4, the first set of models labeled "preliminary screening models" are the least sophisticated models—they require the least extensive input data and are therefore expected to produce the least accurate results. To prevent the rejection of good candidates because of inaccuracies in these models, candidates at this level should be eliminated according to the least strict screening tolerances. As the sophistication (and hence accuracy) improves with the intermediate and advanced evaluation models, the screening tolerances represented by the diamond shapes would likewise decrease appropriately.

A parallel demonstration study [12] used the logic embodied in Figure 4 (preliminary screening and intermediate evaluation models only) to identify the best existing gun propellant for a real gun system with user requirements. In this work, the user-supplied requirements included the maximum pressure limitation and minimum muzzle energy required by a propelling charge for a Navy 5-in, 54-cal. gun. A candidate set of 10 existing propellant formulations representing single, double, triple-based, and composite nitramine propellants was used for the down-select procedure. All combustion properties of this list of propellants are known. The procedure began by assessing environmentally unacceptable ingredients in the propellants—this eliminated two candidates. Thermodynamic property information was obtained from existing literature to assess ideal performance (i.e., muzzle velocity assuming constant maximum pressure during the firing). These estimates allowed a further culling of candidates. Additional unsuccessful candidates were eliminated from the next stage of screening, which is a calculation of interior ballistics performance assuming propellant grain design. At the end of the exercise, the user was left with only a few candidates for further study. At this stage, users can rank these candidates according to their specifications, and more advanced models can be employed to make the final suitability assessment. Thus, this exercise illustrated how the procedure outlined in Figure 4 can be used to reduce the waste stream in the formulation process, while continuing to meet the performance objectives for the gun.

The task now remains to transition this procedure from an idealized concept into a working methodology. Each of the boxes in Figure 4 represent an opportunity to perform a theoretical analysis in lieu of more costly testing. Many of the models described are under development; however, there are many more that need to be developed. For example, the success of the parallel

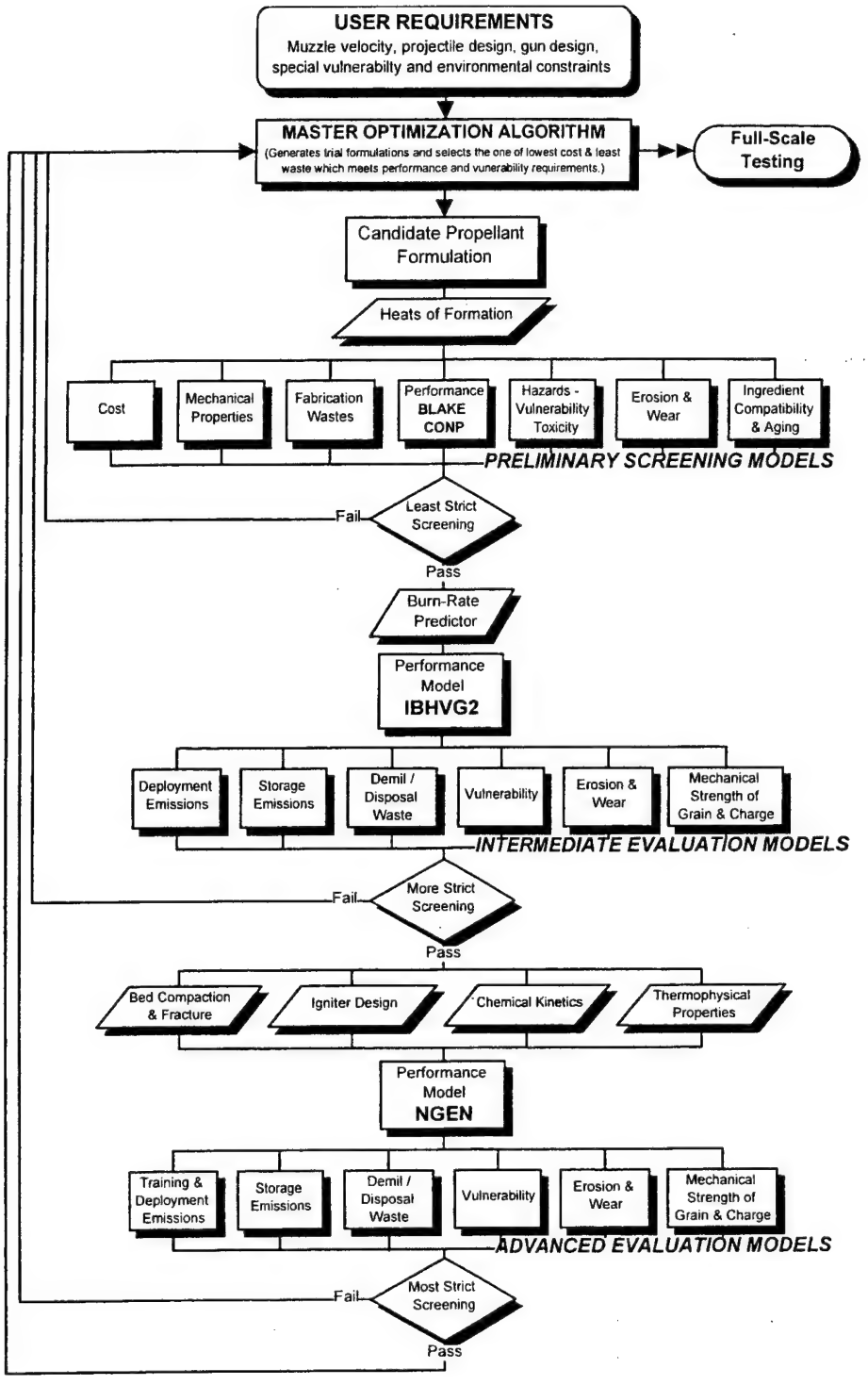

Figure 4. Flow Chart Illustrating the Progressive Winnowing of Propellant Candidates Through a Hierarchy of Models of Increasing Sophistication.

Table 4. Identification of Codes Used in Figure 4

Code	Description	Reference
BLAKE	Equilibrium thermochemistry	[13]
CONPRESS	Constant-pressure ideal gun	[14]
IBHVG2	Lumped-parameter interior ballistics	[15]
XNOVAKTC	Quasi-1-D interior ballistics with flamespreading	[8, 9]
NGEN	2-D/3-D advanced interior ballistics	[16, 17]

exercise was completely dependent on knowledge of the toxicity of the ingredients and knowledge of the combustion properties (such as burning rate, etc.) to perform the screening tests. For notional materials that might be developed for advanced propulsion concepts, this information will not be readily available, and a need exists for predictive models of such. Also, the current models do not accurately predict product emissions from the gun into the atmosphere after gun firing events, which would be an important factor in an environmentally driven development procedure. The most that current models can do is assume that the combustion products are in thermal equilibrium, a situation that may not exist in a gun-firing environment. This deficiency could be remedied by enhancing existing interior ballistics codes to calculate finite rate chemistry at the muzzle. The parallel demonstration also makes use of previously measured burning rates. First-principles burning rate models are under development at ARL to remove dependency on closed-bomb and strand-burner measurements, which requires fabricating any new propellant and synthesizing any new ingredient. If models are developed for all of the boxes in Figure 4, one could replace the first six steps of Figure 3 could be replaced by the hierarchical evaluation models of Figure 4 to achieve even higher cost savings than suggested by Table 3. This end goal is illustrated by the new charge development chart in Figure 5, where all of the models and logic of Figure 4 are represented by the box termed "Master Optimization Algorithm." Thus, Figure 5 represents the full measure of streamlining that might be achieved by fully implementing the science-based design approach. The savings in time and money implied by a comparison of Figure 5 to the traditional approach of Figure 2 is dramatic.

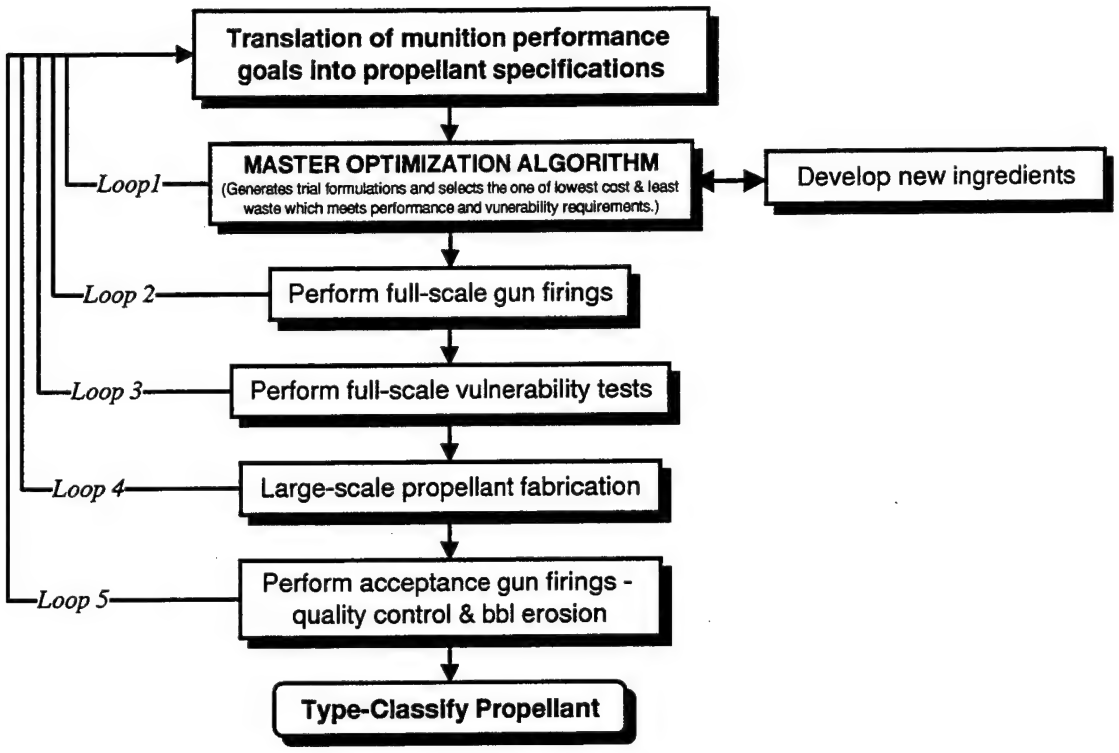

Figure 5. Simplification of Propelling-Charge Development Possible With Full Implementation of Science-Based Design (Compare to Figure 2).

This report has not discussed developing new propellant ingredients, energetic materials, and polymeric binders. It may well happen that performance objectives cannot be met with a propellant made from existing ingredients. Although represented in Figures 1–3 as a single box, there is a similar nested-loop procedure required to develop these. Ingredient development can likewise benefit from strong theoretical guidance during its early phases. Research efforts at ARL are addressing a number of relevant areas such as theoretical chemistry, detonability, and thermophysical properties of polymers. Theoretical chemistry methods can be used to predict properties of novel materials and determine whether a species is stable. These methods can also be used to guide experimental synthesis by predicting favorable reaction routes. In fact, these methods would reduce the need for chemical synthesis, a potentially costly and time-consuming step.

Implementing a science-based approach to propellant formulation will not be trivial or without its own considerable cost and delay. For example, the range of chemistry and physics involved in interior-ballistic phenomena is daunting. Interior-ballistic codes have long been under active

development at ARL. The most advanced code in use is NGEN [14, 15]. This code treats the entire interior-ballistic cycle, from the dispersal of the igniter gases, to flame spreading among the individual propellant grains that make up a propelling charge, to the motion of the projectile down the gun barrel. Descriptions of the full boundary layer flow in and between these grains is not practical, so temporal and spatial averages over this microstructure are effected using mixture theory. This approach necessitates using phenomenological correlations to describe some basic physical interactions, such as drag and heat transfer. While the current correlations seem to work well for a wide range of ballistic problems in artillery and tank weaponry, the demand for ever higher performance may expose new regimes where existing correlations or even the mixture-theory approach itself fails. Should this occur, considerable theoretical work may be required before these ballistic regimes could be modeled accurately. On the other hand, an experimental trial and error approach, in addition to being inefficient and costly, may simply fail.

A rigorous theory of isolated propellant combustion is not yet attainable, largely because of the embryonic state of the theory of reactions in the condensed phase. Even in the gas phase, where both experimental and theoretical techniques exist to treat virtually any reaction, many reactions are poorly known, and remedying these data deficiencies may prove to be both expensive and time consuming. On the other hand, we are at an opportune time in history when the maturation of powerful scientific tools (such as density-functional theory for computing quantum structure of large molecules, molecular dynamics with realistic force fields, and unprecedented computer resources) give confidence to an optimistic prognosis for achieving these goals.

Developing models to fill the screening and evaluation boxes in Figure 4 represents a very great scientific challenge. However, a technically sound and systematic approach to developing the needed models should lead inexorably toward the ultimate goal and provide valuable partial guidance along the way. In any event, the simple simulations presented in this report underscore the unworkability of applying the traditional trial-and-error development approach with the added burden of considering life-cycle costs. Employing modeling and simulation to the early development phases can achieve impressive reductions in cost and time. In view of the national need to provide ever stronger

weapons capabilities in the face of declining resources, there appears to be little choice but to pursue a science-based strategy to minimizing these life-cycle costs. Again echoing the words of the Quadrennial Review, "We not only have the opportunity to change, we have the requirement to change."

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The traditional approach to developing propellants for specific gun applications relies heavily on trial and error. Candidate formulations must be made in small quantities and subjected to burning-rate measurements and small-scale vulnerability assessments. If the properties of these candidates fail to meet expectations, the process must be repeated. This approach, while historically unavoidable, is obviously inefficient in time and expense and can generate considerable waste streams associated with unsuccessful formulations. With added considerations of life-cycle costs, including environmental impact at all stages of development, use, and disposal, this traditional approach becomes increasingly unworkable. This report proposes a new approach that makes maximal use of scientific understanding embodied in models during the early phases of the propellant-development cycle. Simple simulations show that this strategy can have a significant impact on the overall costs of the development process. In analogy to the Department of Energy (DOE) program to convert the nuclear-weapon stewardship from testing-based to science-based, we term the new approach science-based design. This new approach will require concentration and leveraging of resources toward the most critical early-phase development steps; with the reality of declining resources, it may be the only credible strategy to reconcile the need for higher-performance weapons.

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